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ELECTRONIC STRUCTURE OF POLYATOMIC MOLECULES.

(10) by J. C. Slater.

(5) Massachusetts Inst~~itute~~ of Tech~~nology~~,
Cambridge, ~~Mass.~~

(15) Contract ~~No.~~ AF 19(628)-356,
Proj~~ect~~ 6694,
Task 669405

FINAL REPORT

July 31, 1964

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Abstract

Progress in the calculation of the electronic structure of polyatomic molecules in the Solid-State and Molecular Theory Group and the Cooperative Computing Laboratory at M. I. T. is described. This includes the preparation of a system of programs called the POLYATOM system, which allows one to specify the types of atoms and their positions in a polyatomic molecule, and which then proceeds to compute the various molecular integrals required for solving the quantum-mechanical problem of the electronic structure of this molecule, to combine these integrals in a suitable way, and to end up with a calculation of the electronic wave function. Applications of early versions of this method to the structure of benzene and of ethylene are described, and examples of more complicated molecules which have been discussed by the method are described.

1. Introduction

The objective of the present research, as originally stated, was to accomplish the following:

Investigations directed toward the determination of the electronic structure of organic molecules and semiconductors. This determination is to be done from a theoretical approach using the methods of quantum mechanics. This work will include, but not be limited to, the following:

(a) Molecules such as benzene, napthalene and anthracene will be studied and these stuides will be extended to systems such as coronene if the results on less complicated molecules are promising.

(b) Other molecular systems are to be investigated if such investigations will assist in the studies outlined in (a) above.

(c) Non-empirical methods are to be employed in finding numerical solutions to the Schrödinger equation with as few approximations as possible.

(d) Based upon the results of the calculations, conclusions are to be made concerning the distribution of the electrons in the energy levels, the susceptibility of these electrons to optical and thermal excitations, and the criteria upon which chemical synthesis can be based in order to optimize the use of the various compounds for photoconduction or photovoltaic effects.

The contract AF 19(628)-356, for which this is a Final Report, was a continuation of Contract 19(604)-8445, dated May 1, 1961, on which a Final Report was submitted on April 30, 1962. The present contract formed a continuation of this earlier work, and covered the period May 1, 1962--April 30, 1964.

The fundamental purpose of the research was to develop methods of carrying out a priori calculations of polyatomic molecules, particularly of simple organic molecules, which would contribute to our knowledge of the method of studying more complicated organic molecules, and the crystalline forms of organic substances. It was recognized at the outset that this was a very extensive task, and that only the earlier stages were likely to be carried through in the immediate future. The first specific molecule undertaken for study was benzene, the simplest example of the aromatic compounds. It was hoped that methods developed for that problem would be applicable in other cases, and that these methods could be tested by applying them to simple molecules before undertaking more complicated problems.

The following workers were associated with the contract:

Dr. J. W. Moskowitz
Dr. M. C. Harrison
Dr. B. T. Sutcliffe

The work was done in close contact with Prof. M. P. Barnett, Dr. I. G. Csizmadia, R. M. Pitzer, D. E. Ellis, J. P. Wright, and other members of the Solid-State and Molecular Theory Group and the Cooperative Computing Laboratory at M. I. T. This group of workers, under the direction of Prof. Barnett, was concerned with the general problem of developing computational methods of handling polyatomic molecules. We shall start our discussion with a description of the computational methods developed under this program, partly under the sponsorship of the contract being reported on, partly under grants from the National Science Foundation and the National Institute of Health, and then shall go on to the work on specific molecules.

2. General Computational Methods for Polyatomic Molecules

There are two main types of computation involved in the a priori calculation of the electronic structure of a polyatomic molecule. First, one needs so-called two-center, three-center, and four-center integrals between atomic orbitals located on various atomic sites. Two different mathematical approaches to the description of the atomic orbitals are in common use. One of these uses exponential functions times polynomials (sometimes denoted as Slater-type orbitals), the other uses Gaussian functions times polynomials. The exponential type of approximation requires fewer terms to approximate the atomic orbital adequately, but the formulas for the integrals are much simpler with the Gaussian orbitals, and it is an open question which method leads to the final answer in a simpler fashion. We have followed through with both methods in our work, and have found it useful to be able to check the accuracy of calculations made by one method by repeating them by the other. Calculations of the integrals using the exponential type of atomic orbitals are made by a method to which the names of Barnett and Coulson are attached, while those using Gaussian orbitals use a method originated by Boys. The general methods of calculation of integrals by either scheme are outlined in the chapter by Prof. Barnett in "Methods in Computational Physics", edited by B. J. Alder, S. Fernbach, and A. Rotenberg, Academic Press, Inc., New York, 1963[1].

The other type of calculation involved is that of combining the required integrals, sometimes involving hundreds of thousands of terms, into the expression for the final answer. This process is so complicated that it is practically necessary to carry it out on the digital computer. In fact, every step of the process of calculating the structure of a polyatomic molecule is so extensive that the aim of the group has been to mechanize the whole thing, producing a program whose input would be a statement of the atoms involved and their nuclear positions, and whose output would be a complete solution of the electronic problem involved in the molecule. During the period covered by this contract, great progress has been made toward both types of calculation, part of the work having been done under the present contract.

As for the multicenter integrals, the integrals involving exponential-type atomic orbitals are computed at present by a set of programs that are available as self-contained binary decks to be run under the standard IBM Fortran Monitor system on any 709/ 90. These decks may be used to compute:

1) Three-center resonance integrals involving K and L shell orbitals.
2) Three-center Coulomb integrals (aabc) involving K and L shell orbitals.
3) Three-center exchange integrals (abac) involving K and L shell orbitals.
4) Four-center integrals involving s-orbitals of principal quantum number $n < 12$.

Further less completely developed programs compute 4-center integrals between 2p orbitals. In addition, a package is available for computing all integrals involving K and L shell orbitals in a Gaussian basis according to the method of Boys and co-workers[2].

In order to surmount the data processing problem inherent in any molecular computation a system of programs has been written by the various members of the group, called the POLYATOM system, described by M. P. Barnett,[3] and in more detail in Technical Note No. 36 of the Cooperative Computing Laboratory of M. I. T., by I. G. Csizmadia, M. C. Harrison, J. W. Moskowitz, S. Seung, B. T. Sutcliffe, and M. P. Barnett. There will be further Technical Notes regarding various aspects of this system. The POLYATOM system involves several major blocks which are listed below. It will be possible to use these in a fully automatic manner or under namual control, by the provision of appropriate master programs and linking parameters. The system is coded in Fortran for the IBM 7094 computer. The main blocks of the initial system are as follows:

1. An input program to store the nuclear coordinates and orbital parameters of the basis functions with their transformation properties.
2. An integral list generator, to list the names of the integrals between basis functions that are needed. This list omits the names of zero integrals, and associates the names of integrals that are equal due to symmetry.
3. An integral evaluation program, that will compute the necessary integrals in either a Gaussian or Slater orbital basis.
4. A SCF (self-consistent-field) program. Several SCF programs have been written to deal with open and closed shell systems and basis sets of different sizes.
5. A program to transform one and two electron integrals from one basis set to another.
6. A configuration interaction package based on the codetor notation of Boys.
7. A program to form density matrices, dipole moments, and related physical properties.

Particular attention has been given to the design of calculations that can be repeated, extended, or modified by other workers. Elaborate checking techniques have been built into the programs to ensure that the results really do correspond to the mathematical formulations that are used. It is intended to do extensive preliminary calculations on simple atomic and molecular species in order to gain experience before attacking the more complex systems. Some of these calculations will be described in later sections. The POLYATOM system as presently written makes provision for a set of 50 basis orbitals.

3. Calculations on Specific Molecules

The benzene molecule was first treated by Goeppert-Mayer and Sklar[4] as a system of six $2p\pi$ electrons mutually interacting and moving in the potential field of the molecular core. The core consists of the carbon and hydrogen nuclei, the 1s atomic orbitals of the carbon atoms, and the molecular orbitals which describe the single bonds. The validity of the strict separability of the sigma and pi electrons has been examined by Lykos and Parr[5]. They conclude that a quantum mechanically meaningful H_π can be defined for the pi electrons such that the expectation value of the operator over a wave function for the π electrons alone gives the pi electron contribution to the total energy including sigma-pi coulomb and exchange interactions. The assumed form of the sigma wave function has not been the subject of extensive investigation. The Goeppert-Mayer and Sklar potential is then derived from the additional assumptions: (1) The contributions to the core potential coming from the hydrogen nuclei and the electronic distributions surrounding them can be neglected. (2) The part of the potential coming from the carbon nuclei and the electronic distribution surrounding them can be approximated as the potential due to carbon atoms in their valence states minus the charge distribution of an electron in a π orbital. (3) All exchange terms with the core electrons are to be neglected.

The molecular orbitals for the six π electrons are written in the form of Bloch sums or symmetry orbitals which may be comveniently designated a_{2u}, b_{2g}, e_{1g}, and e_{2u} respectively. In the ground A_{1g} state a_{2u} and e_{1g} are fully occupied. Goeppert-Mayer and Sklar examined the excited states which differ from the ground state by having one electron lifted into e_{2u}, leaving a hole in e_{1g}. The symmetries of these states are $^{1,3}B_{1u}$, $^{3}B_{2u}$, and $^{1,3}E_{1u}$. In calculating the energies all three and four center molecular integrals were neglected. The calculations have been extended by Roothan and Paar,[6] Niira,[7] and particularly by Parr, Craig, and Ross,[8] who introduced limited configuration interaction into the computation. In addition the benzene molecule has been studied in the alternant molecular orbital approximation by Löwdin, Pauncz, and de Heer[9]. The above calculations have at best been qualitatively successful.

A study of the excited energy levels of the benzene molecule, using the core approximation, was carried out under the contract by Dr. Moskowitz and

Prof. Barnett.[10] This employs a larger configuration interaction than has been used previously for the molecule, as well as an accurate computation of all multicenter integrals. As a preliminary to this calculation, Dr. Moskowitz made a study of the H_6 ring in the molecular orbital and alternant molecular orbital approximation.[11] This carried further a study of the H_6 molecule which had been made by Mattheiss,[12] in the Solid-State and Molecular Theory Group. The configuration interaction problem of the π electrons in benzene is formally equivalent to this problem of H_6, but it involves more complicated integrals. The H_6 case was used by Moskowitz to investigate the applicability of the alternant molecular orbital and second-order perturbation theory approximations to such a problem.

The most striking feature to emerge from the benzene calculation (Ref. 10) is the fact that the better the wave function, the smaller the multiplet separations. The singlet-triplet separation is 2.514 eV for the full configuration interaction treatment, which has made the agreement with the experimental value of about 3.8 eV poorer than was found by earlier, less accurate calculations. This does not prove that electron correlation effects are unimportant, but that there is an essential defect in our present quantitative approach to the quantum chemistry of conjugated hydrocarbons.

A possible remedy would be to include the sigma electrons explicitly. Due to the difficulty of the benzene problem, a pilot calculation has been undertaken by Drs. Moskowitz and Harrison[13] on the ethylene molecule, using a Gaussian basis. The results indicate that the Gaussian basis provides an adequate representation of the molecular wave function. In the case of ethylene the concept of sigma-pi separation seems to be adequate. In fact, the pi electrons are relatively insensitive to the inner core orbitals. The calculation of the electronic excitation energies is still far from satisfactory.

Since carrying out this work on ethylene, Drs. Moskowitz and Sutcliffe, now working at New York University, have extended the basis set for ethylene, obtaining a final energy for the molecule of -77.92121 AU. They feel that this is quite close to the Hartree-Fock limit, and gives a "molecular extra correlation energy" of 0.308 AU. This may be compared to the semi-empirical value of 0.401 AU predicted by Clementi. They are working now on a large configuration interaction study of the ethylene molecule.

In addition to these two molecules, benzene and ethylene, which have been studied under the contract, memebers of the Solid-State and Molecular Theory Group have applied the methods which have been developed for polyatomic molecules to several other molecules. The water molecule has been further studied, partly to test the methods. The most ambitious case to which the methods have been applied is formyl fluoride, a prototype of a number of more complicated and interesting molecules. The success which has been obtained in these calculations, though they were not carried on directly under the present contract, shows that the methods which have been developed over the past several years are now capable of producing very valuable results in the study of the electronic structure of polyatomic molecules. Thus the primary purpose of the present contract has been achieved, though it still remains for the future to apply these methods to various more complicated problems.

4. Future Prospects for Research in Polyatomic Molecules

At the time of writing this report, all of the persons who have been associated with the project have left the Solid-State and Molecular Theory Group, except for D. E. Ellis, who is still working for his doctor's degree. Only M. C. Harrison in addition is still at M. I. T., but in quite a different project. Thus the type of research which is reported on here has largely stopped, as far as M. I. T. is concerned. This does not mean, however, that the line of research will not continue in the future, or that the work done under the contract will be lost.

Drs. Moskowitz and Sutcliffe have gone to New York University, where Moskowitz has become Assistant Professor of Chemistry. There they are continuing work along the same lines, under a new contract with the Air Force Cambridge Research Laboratory. Part of the work mentioned in this report on ethylene has been done under this new contract. They have every intention of continuing research dealing with the same type of problem, thus approaching more nearly to the long-range goal of the present contract, namely the understanding of the electronic structure of organic semiconductors.

Prof. Barnett has gone to the Computer Unit of the University of London. Among the many projects which he expects to undertake there is a continuation of the work on polyatomic molecules which was begun here. Dr. Csizmadia expects to spend some time in the group of Prof. Barnett in London, working on these problems, before taking a permanent post in Canada. Part of the work relating to the programs for carrying out calculations on polyatomic molecules has already been reported in Technical Notes of the Cooperative Computing Laboratory at M. I. T., and further portions will be reported in the future. In addition, many parts of the programs are being made avialable through the Quantum Chemistry Program Exchange at Indiana University.

5. Publications

Publications directly resulting from contract:

J. W. Moskowitz, Study of the H_6 Ring in the Molecular Orbital and Alternant Molecular Orbital Approximation, J. Chem. Phys. 38, 677 (1963)

J. W. Moskowitz and M. P. Barnett, Pi Electronic Structure of the Benzene Molecule, J. Chem. Phys. 39, 1557 (1963)

J. W. Moskowitz and M. C. Harrison, The Ethylene Molecule in a Gaussian Basis. I. A Self Consistent Field Calculation, submitted to J. Chem. Phys.

Related Publications from Solid-State and Molecular Theory Group:

M P. Barnett, The Evaluation of Molecular Integrals by the Zeta Function Method, chapter in "Methods in Computational Physics", Vol. II, pp. 95-153, Academic Press, 1963

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I. G. Csizmadia, B. T. Sutcliffe, and M. P. Barnett, A Group Orbital Study of Lithium Hydride, submitted to Can. J. Chem.

C. S. Roberts, Interaction Energy between a Helium Atom and a Hydrogen Molecule, Phys. Rev. 131, 203 (1963)

B. J. Woznick, Self-Consistent Field Calculation of the Ground State of Methane, J. Chem. Phys. 40, 2860 (1964)

Contributions to Quarterly Progress Reports of Solid-State and Molecular Theory Group, M.I.T., Nos. 45-52, dealing with Related Topics

Techniques of Calculation

M. P. Barnett and M. C. Harrison, Automatic Calculation of SCF Wave Function, 47, 121 (1963)

J. P. Dahl and M. P. Barnett, Expansion Theorem for Solid Spherical Harmonics, 48, 53 (1963)

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D. E. Ellis, Molecular Calculations 46, 148 (1963)

D. E. Ellis, Molecular Integrals over Slater Orbitals, 48, 47 (1963); 49, 85 (1963)

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B. T. Sutcliffe, Configuration Interaction, 50, 44 (1963)

J. P. Wright, Three-Center Coulomb and Exchange Integrals, 47, 123 (1963)

J. P. Wright, Four-Center Molecular Integrals, 48, 52 (1963)

J. P. Wright and M. P. Barnett, The b and c Coefficients that are Used in Some Expressions for Multicenter Molecular Integrals, 50, 27 (1963)

J. P. Wright, Four Center Integrals--Gaussian and Slater Functions, 50, 35 (1963)

Results of Calculations

M. P. Barnett, I. Csizmadia, M. C. Harrison, J. W. Moskowitz, and B. Sutcliffe, Aromatic and Related Molecular Calculations, 47, 117 (1963)

I. Csizmadia, M. C. Harrison, and B. T. Sutcliffe, Non-Empirical LCAO-SCF Calculation of Formyl Fluoride with Gaussian Atomic Orbitals, 50, 4 (1963)

M. C. Harrison, SCF Calculation on Neon, Using Gaussian Functions, 49, 74 (1963)

M. C. Harrison, SCF Calculations on H_2O, Using Gaussian Functions, 50, 20 (1963)

J. W. Moskowitz, Benzene, 45, 111 (1962); 47, 117 (1963); 48, 43 (1963)

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C. S. Roberts, Inelastic Scattering from a Diatomic Molecule, 47, 86 (1963)

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B. J. Woznick, Methane, 45, 110 (1962); 47, 107 (1963)

Technical Notes of the Cooperative Computing Laboratory, M. I. T., Related to Work of the Contract

No. 23. Some Programs to Evaluate Multicenter Integrals by the Zeta Function Method, R. M. Pitzer, J. P. Wright, and M. P. Barnett

No. 26. Surface Harmonic Expansions of Products of Cartesian Coordinates, A. B. Otis, Jr. and M. P Barnett

No. 31. Computer Generated Formulae for the $e^{k,j,i}_{x,w}$ Coefficinets of Theoretical Chemistry, H. D. Wactlar and M. P. Barnett

No. 32. A Group Orbital Study of Lithium Hydride--Supplementary Material, I. G. Csizmadia, B. T. Sutcliffe, and M. P. Barnett

No. 36. The POLYATOM System, by I. G. Csizmadia, M. C. Harrison, J. W. Moskowitz, S. Seung, B. T. Sutcliffe, and M. P. Barnett, Part I. Description of Basic Subroutines, by M. C. Harrison

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Mass. Institute of Technology, Cambridge, Mass.
ELECTRONIC STRUCTURE OF POLYATOMIC MOLECULES by J.C. Slater. Air Force Cambridge Research Laboratories, Bedford, Mass. Final Report-Number AFCRL 64-458. 16 pages. July 1964.
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Progress in the calculation of the electronic structure of polyatomic molecules is described. This includes the preparation of a system of programs called the POLYATOM system, which allows one to specify the types of atoms and their positions in a polyatomic molecule, and which then proceeds to compute the various molecular integrals required for solving the quantum-mechanical problem of the electronic structure of this molecule, to combine these integrals in a suitable way, and to end up with a calculation of the electronic wave function. Applications to the structure of benzene, ethylene, and more complicated molecules are described.

1. Theoretical calculations-polyatomic molecules

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